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ON THE APPLICATION OF THERMODYNAMIC METHODS TO THE ANALYSIS OF QUANTUM STATES

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The presented work is devoted to the problem of stability of quantum systems. There are investigated possibilities of the statistical entropy using as a criteria for the equilibrium. The harmonic oscillator is used as an example for classical and quantum theories. It's shown that from thermodynamics point of view the quantum distributions are more advantageous than classical ones.

Keywords: stability, quantum systems, statistical entropy, criteria for the equilibrium, quantum distributions.

In this article we start an investigation and analysis of the stability problem of some quantum systems. This intention is motivated by the question of stability of wave packets. We suppose that as ones quantum states are more stable than others then it can be a course for existing of dynamically stable wave packets [1]. Usual approaches of quantum mechanics are not proper enough for our aims. So we intend to check the stability conditions made into thermodynamics for using in quantum theory. Really the thermodynamics in the statistical representation is the probabilistic theory like the quantum mechanics. It's mean that they can have intersections and analogies. This idea isn't original one and there are many publications worked up this. For example paper [2] is devoted to investigation of open quantum systems or many others which can be easy found in science bases. But our gain is using thermodynamic methods to single particle systems and this is main feature of our approach. What we need very hard in this case is the caution and accuracy. We have rights to use the thermodynamic derivations for statistic ensembles, but not for many particle systems.

Quantum mechanics the theory is intended for consideration of systems with one or few particles. All information about the system is contained into the wave function. A density of the probability of some physical states can be found as

$$\rho = \psi^* \psi .$$

Statistical physics considers systems of many particles and ρ is the density of probability to find the system in given state too. So both quantum mechanics and statistical physics consider the densities of probability of states. We reckon that links between statistical physics and thermodynamics let us the possibility to use the phenomenological thermodynamics laws for some aspects of quantum theory. More concretely we are interesting in the stable conditions for probabilistic systems. The main role of the stable criteria for closed systems belongs to entropy.

Namely, closed system is stable if entropy S has a maximum value. Von Neuman's definition of entropy

$$S = - \int \rho \cdot \ln \rho d\Gamma$$

is the most convenient expression for the investigation. The mathematician determination of the entropy in one-dimensional case has a view

$$S = -\int \rho \ln \rho dx, \quad (1)$$

where $\rho = \rho(x)$.

Let us suppose, that S is the maximum for a stable state in mechanics. In order to check it let consider the classical harmonious oscillator:

$$x = A \cos(\omega t + \varphi_0)$$

It is not difficult to find that probabilistic distribution for this case has a view:

$$\rho(x) = \frac{1}{\pi \sqrt{A^2 - x^2}}. \quad (2)$$

Inserting this expression into (1),

$$S = -\int_{-A}^A \frac{1}{\pi \sqrt{A^2 - x^2}} \ln \frac{1}{\pi \sqrt{A^2 - x^2}} dx,$$

the replacement $\frac{x}{A} = \cos \varphi$, and some transformations lead to the integral

$$S = \frac{1}{\pi} \int_0^\pi \ln(\pi A \sin \varphi) d\varphi.$$

The integral of such view is presented in the handbook [3]:

$$\frac{1}{2} \int_0^\pi \ln(\sin x) dx = -\frac{\pi}{2} \ln 2.$$

So, we have got the following expression for the entropy:

$$S = \ln \frac{\pi A}{2}. \quad (3)$$

The result is strange for physics, because it depends on a scale of a space. It is normal from mathematical point of view since a change of the entropy S can be calculated. But the result in physics is necessary to agree with the third law of thermodynamics, which suppose an absolute character of entropy. In order to find an expression for the entropy that does not depend on a scale, one need to start from the expression for discrete case:

$$S = -\sum_i W_i \ln W_i.$$

Let take W_i as the expression:

$$W_i = \rho_i \Delta x_i,$$

where every $\Delta x_i = \Delta x$ are identical.

After inserting it into the previous expression, we get to

$$S = -\sum_i \rho_i \Delta x \ln(\rho_i \Delta x) = -\sum_i \rho_i \Delta x \ln(\rho_i) - \sum_i \rho_i \Delta x \ln(\Delta x).$$

One can see that $\sum_i \rho_i \Delta x = 1$ and $\lim_{\Delta x \rightarrow 0} \ln \Delta x = -\infty$.

It is meaning that after transition to the continuous distribution ($\Delta x \rightarrow 0$) entropy stands by degenerate one. In order to avoid this, one can be introduced the discreteness of a space.

Let l_0 be the minimum step of the space, then at the condition $A \gg l_0$ we obtain for the entropy besides (3):

$$S = \ln \frac{\pi A}{2l_0} \quad (4)$$

This expression, in contrast to (3), is consistent at formal point of view. Note that introducing of the space discreteness, i.e. manifestation of its discrete properties, leads us to the ideas of quantum mechanics. Really, in this case at low energies the space probability find system should differ from distribution (1) and be similar with quantum distribution:

$$\rho_n = \frac{1}{2^n n! \sqrt{\pi} x_0} e^{-\left(\frac{x}{x_0}\right)^2} H_n^2\left(\frac{x}{x_0}\right) \quad (5)$$

Now let consider the quantum case. According to (5) for the first two stable states we have:

$$\rho_0 = \frac{1}{\sqrt{\pi} x_0} e^{-\left(\frac{x}{x_0}\right)^2}, \quad \rho_1 = \frac{2}{\sqrt{\pi} x_0} \left(\frac{x}{x_0}\right)^2 e^{-\left(\frac{x}{x_0}\right)^2} \quad (6)$$

Calculations due to (1) lead to next expressions for entropy:

$$S_0 = \frac{1}{2} + \ln\left(\sqrt{\pi} \frac{x_0}{l_0}\right), \quad S_1 = C + \ln 2 - \frac{1}{2} + \ln\left(\sqrt{\pi} \frac{x_0}{l_0}\right), \quad (7)$$

where $C = 0,57721566490 \dots$ is Euler's number and l_0 is taken account due to the previous reasoning. Let do the comparison the entropies for classical (S) and quantum cases (S_0 for beginning) and introduce the difference

$$\Delta S = S_0 - S. \quad (8)$$

Let do the calculations for one value of energy. For the ground state of the oscillator $E_0 = \frac{\omega\hbar}{2}$, taken account the classical expression $E = \frac{m\omega^2 A^2}{2}$, we can get to the classical value of the amplitude $A = \sqrt{\frac{\hbar}{m\omega}}$, or $x_0 = \sqrt{\frac{\hbar}{m\omega}}$, as it is denoted in quantum mechanics. Inserting one into (4), (7) and (8) leads to the expression:

$$\Delta S = \frac{1}{2} + \ln\left(\frac{\sqrt{\pi} \cdot x_0 \cdot 2}{\pi A}\right) = \frac{1}{2} + \ln\left(\frac{\sqrt{\pi} \cdot \sqrt{\frac{\hbar}{m\omega}} \cdot 2}{\pi \cdot \sqrt{\frac{\hbar}{m\omega}}}\right) = \frac{1}{2} + \ln\frac{2}{\sqrt{\pi}}.$$

The numerical calculates give us $\Delta S = \frac{1}{2} + 0.69314718 - 0.57236547540 > 0$. It shows that the quantum distribution is more advantageous than classical one due to bigger the entropy. It is not amazing since distribution (6) for ground state has the Gauss character.

Let calculate the same difference for the entropy S_1 :

$$\Delta S_1 = S_1 - S.$$

For the first excited level we have $E_1 = \frac{3\omega\hbar}{2}$ and associated value for the classical amplitude:

$$\frac{3\omega\hbar}{2} = \frac{m\omega^2 A_1^2}{2} \Rightarrow A_1 = \sqrt{3\frac{\hbar}{m\omega}}.$$

So, taking into account (4) and (7) we have:

$$\Delta S_1 = C + \ln 2 - \frac{1}{2} + \ln\left(\frac{\sqrt{\pi} \cdot x_0 \cdot 2}{\pi A}\right) = C - \frac{1}{2} + \ln\left(\frac{4}{\sqrt{3\pi}}\right).$$

Numerical calculations give us

$$\Delta S_1 = C - \frac{1}{2} + 1.386294 - 1.121671 > 0,$$

i.e. we have the same situation, that quantum distribution is more advantageous than classical one if we are appreciating the advantage from the thermodynamic point of view.

Further reasoning meet some difficult for harmonic oscillator. Namely the problems are associated with the deducing of the analytical expression for the entropy of the second level and upper ones. But we think that this problem will be solved by computer methods.

Another problem is associated with our doubts in correctness of the used approach that appeared after analysis of formal features of the equations. Really, it is easy to see the fact that the expression for ρ_0 have the form of the canonical distribution. In classical thermodynamics it corresponds to the system into thermostat, but not closed in energy mean. In such a way, we have to make the conclusion about necessity of consideration the quantum systems as ones in a thermostat. At any case this is looking that for the harmonic oscillator. In the thermodynamics the criteria for stability of such systems is free energy. We think that this is a ground for introduction of similar parameter in quantum mechanics.

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